CRYSCALC

how to calculate a powder diffraction pattern from a .CIF file?

Powder diffraction pattern can be calculated with **CRYSCALC**, using the following general expression :

$$y_i = b_i + \sum_{\mathbf{H}} I_{\mathbf{H}} . \Omega$$

where :

- b_i: background contribution
- y_i: counting at the angular value $2\theta_i$
- $I_{\mathbf{H}}$: integrated intensity of the reflection **H**
- Ω: profile function

Background contribution, type of profile function (pseudo-Voigt or Thompson-Cox-Hastings) as well as profile functions parameters and pattern calculation conditions (incident beam, wavelength, $2\theta_{min}$, $2\theta_{max}$, step and scale factor) are defined in the `cryscalc.ini` ([PATTERN SIMULATION] section).

As in FullProf, background contribution b_i can be described by a polynomial function with a_m coefficients (max. 8th order) :

$$b_i = \sum a_m . (2\theta / BKPOS - 1)^m$$

where `BKPOS` is defined as $(2\theta_{min} + 2\theta_{max})/2$.

Integrated intensity for each reflection is calculated from structural data (space group, cell parameters, atomic positions and adp's) given in a `CIF` file, coming for example from a structural database.

Simplest way to calculate a powder diffraction pattern is to launch **CRYSCALC** in command line with the `CIF` file as first argument and `PAT` keyword as second argument:

```
d:\cifs>cryscalc cif_file.cif PAT
```

Different output files are created:

- `xxx_pat_x.xy`: 2 columns format, with header containing calculation profile conditions and structural data
- `xxx_pat_x.prf`: FullProf format.
- `xxx_pat_x.pdpf`: list of hkl reflections, including 2θ, d_{hkl} and relative intensities. The creation of this file is depending on the value of `create_PAT_PDPF` keyword in the [COMMAND LINE ARGUMENTS] section of the setting file.

If **WinPLOTR** is installed on the computer, `PRF` file is automatically loaded and plotted, unless `plot_PRF=0` in the setting file.

Examples of setting files for a X-ray powder diffraction pattern calculation:

- using a Pseudo-voigt function, without any line broadening :

```
[PATTERN SIMULATION]
pdp_beam = X
pdp_wave = 1.5406
X_profile_U = 0.0055
X_profile_V = -0.0015
X_profile_W = 0.0036
X_profile_eta0 = 0.3
X_profile_eta1 = 0.
X_pattern_step = 0.01
X_pattern_scale = 0.002
X_pattern_background = 50.  32.  24.
X_pattern_Xmin = 0.
X_pattern_Xmax = 150.
profile_function = PV
plot_PRF = 0
particle_sizes = 9999.
strain = 0.
```

- using a TCH function, adding line broadening (towards line profile calculated from given profile parameters) due to 100 Å particles size, and plotting PRF with **WinPLOTR**

```
[PATTERN SIMULATION]
pdp_beam = X
pdp_wave = 1.5406
X_profile_TCH_U = 0.0046
X_profile_TCH_V = -0.001462
X_profile_TCH_W = 0.002734
X_profile_TCH_X = 0.
X_profile_TCH_Y = 0.014
X_profile_TCH_Z = 0.
X_pattern_step = 0.01
X_pattern_scale = 0.002
X_pattern_background = 0.
X_pattern_Xmin = 0.
X_pattern_Xmax = 150.
profile_function = TCH
plot_PRF = 1
particle_sizes = 100.
strain = 0.
```

https://cdifx.univ-rennes1.fr/cryscalc